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FIG. 1  
Procedure for Modeling Complexes

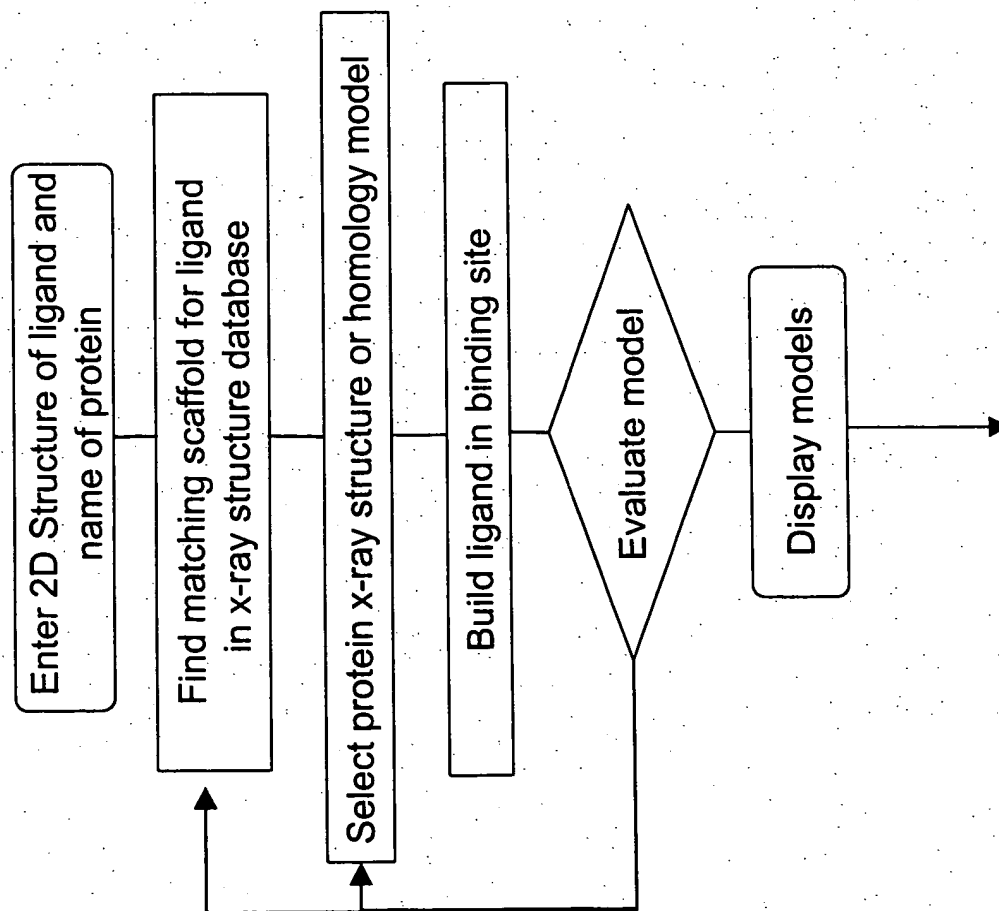


FIG. 2

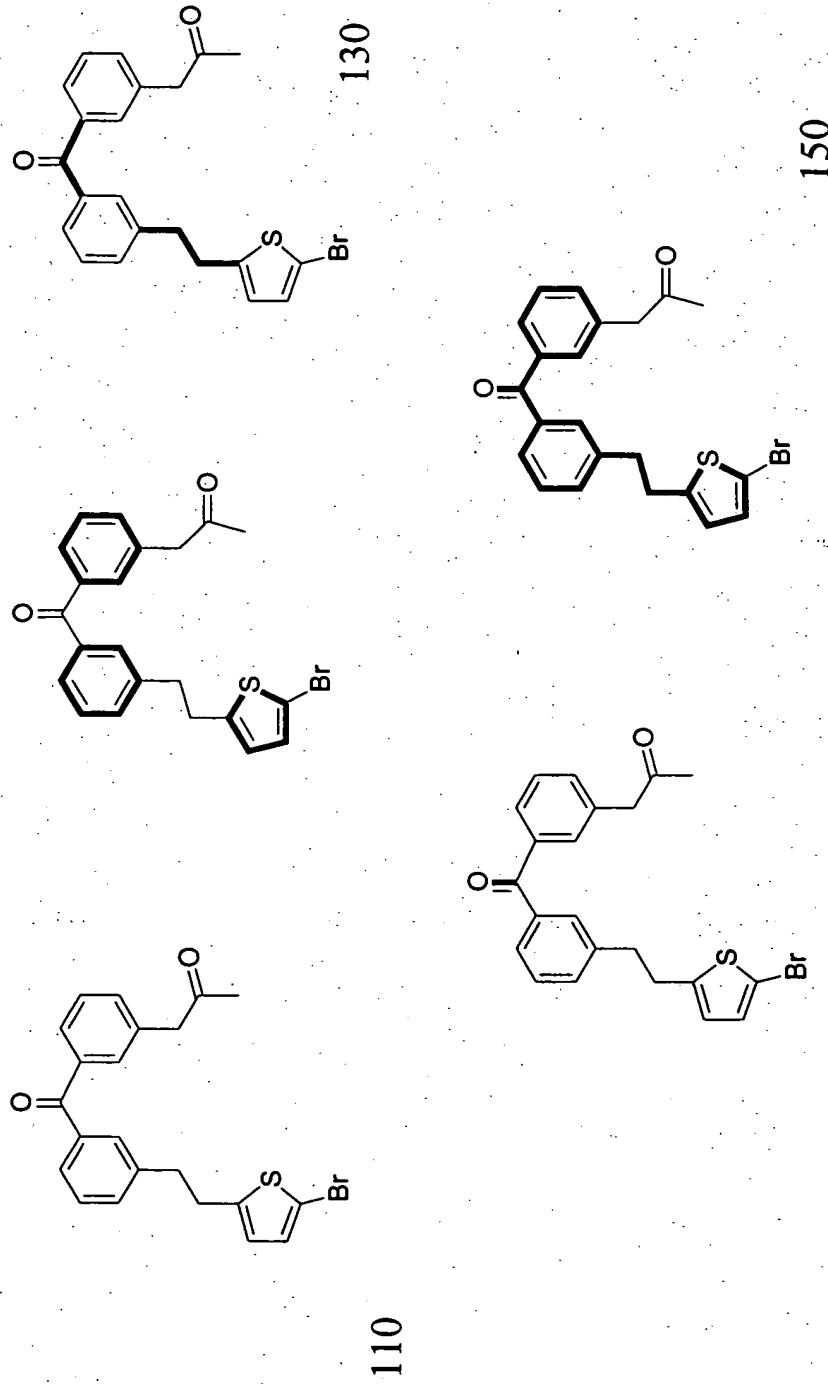


FIG. 3  
Maximum Common Substructure

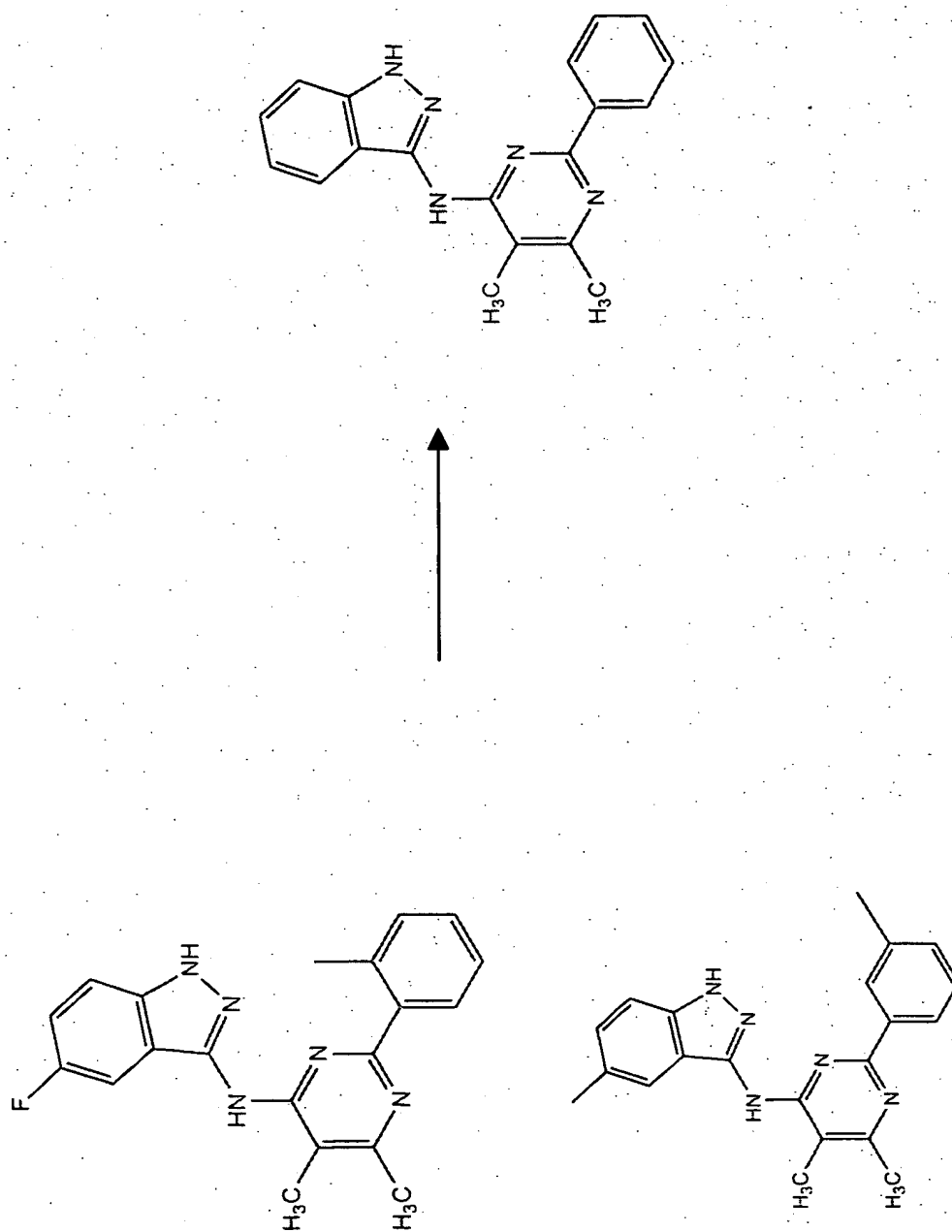
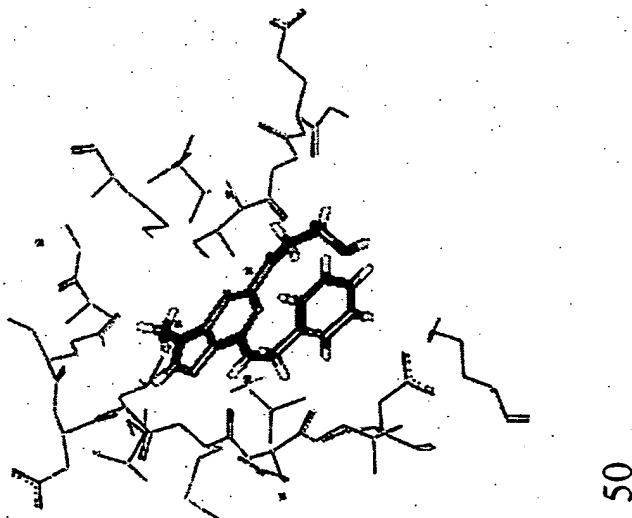
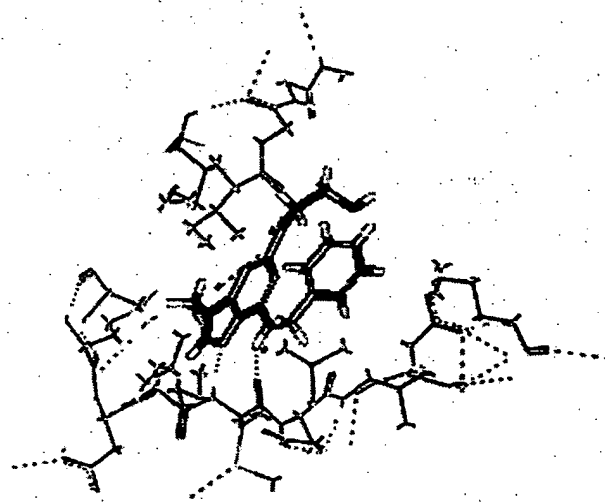


FIG. 4A



60



70

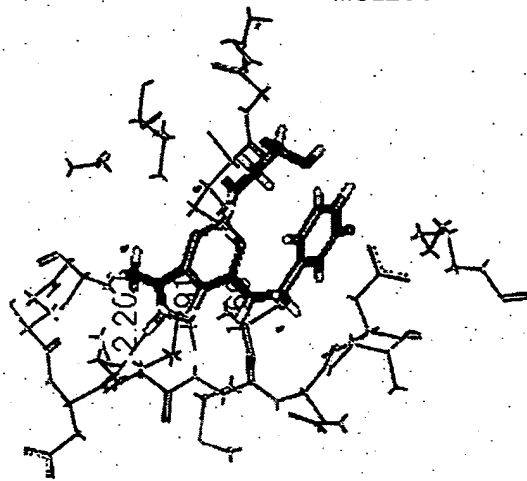
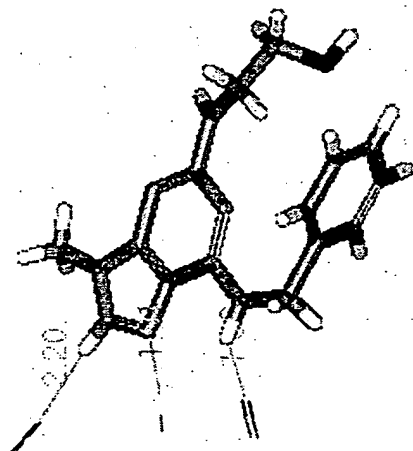
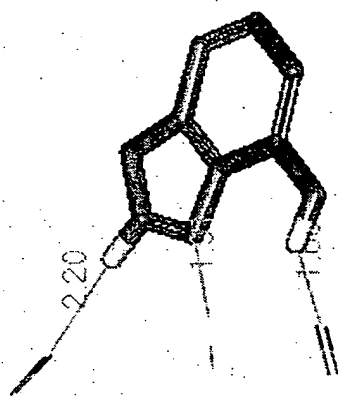


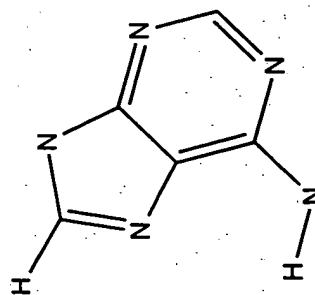
FIG. 4B



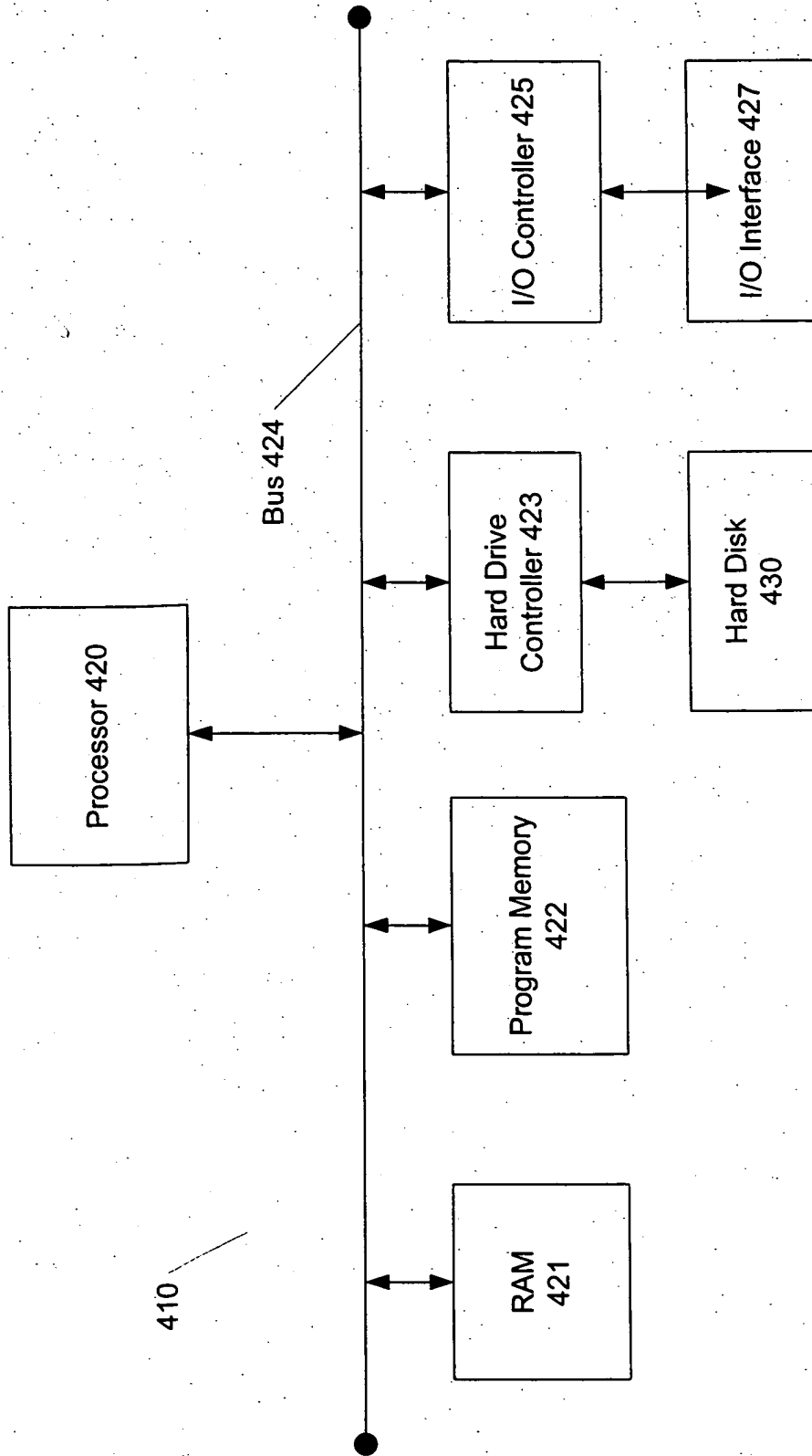
80



90

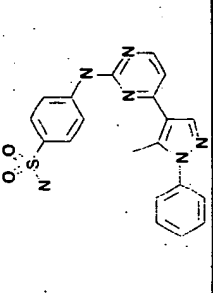
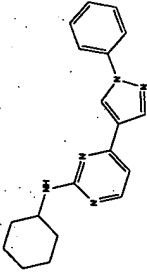
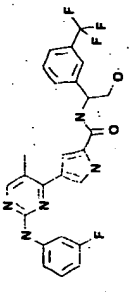
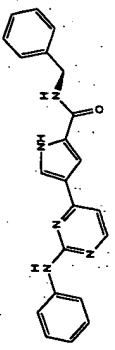
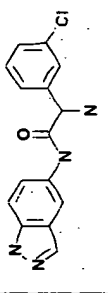
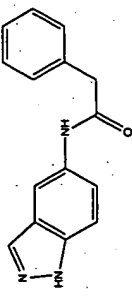
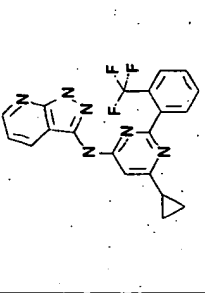
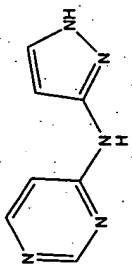


100



**FIG. 5**

FIG. 6

query ligand	protein	scaffold	rmsd (model vs. x-ray) / Angstrom
	jnk3		0.9 – 1.3
	erk2		1.5 – 2.0
	pka(5xm)		1.2
	gsk3β		1.3 – 2.2



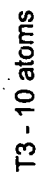
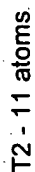
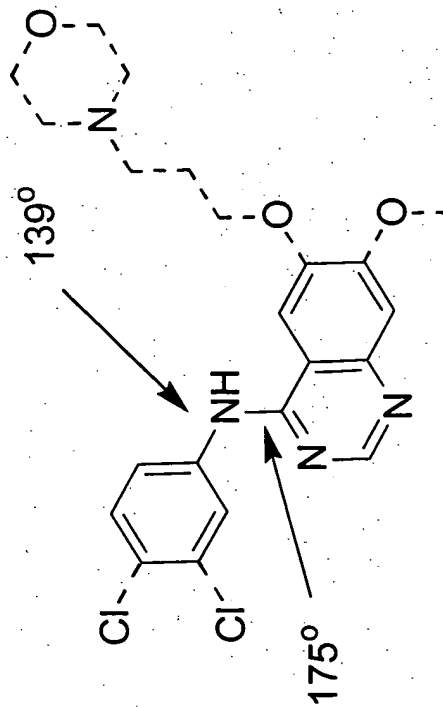


FIG. 8



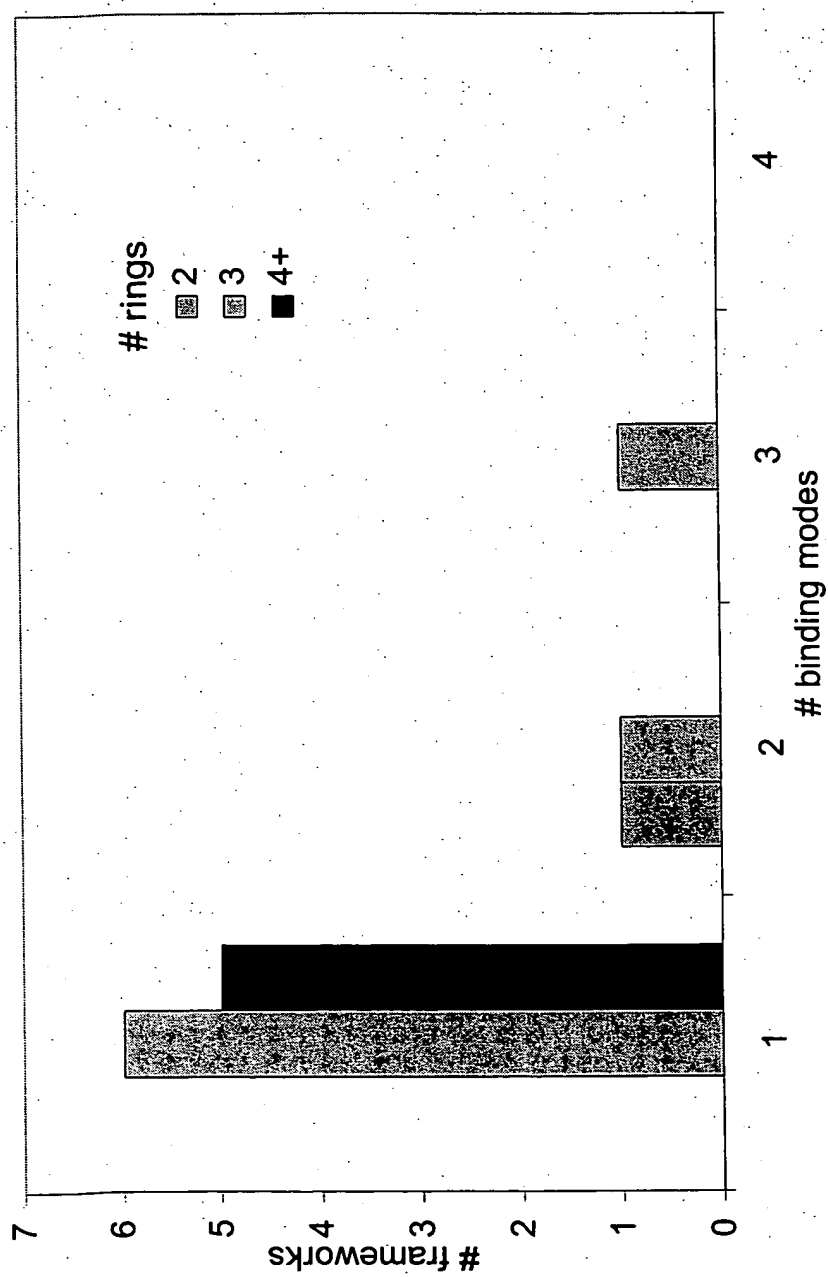


FIG. 9

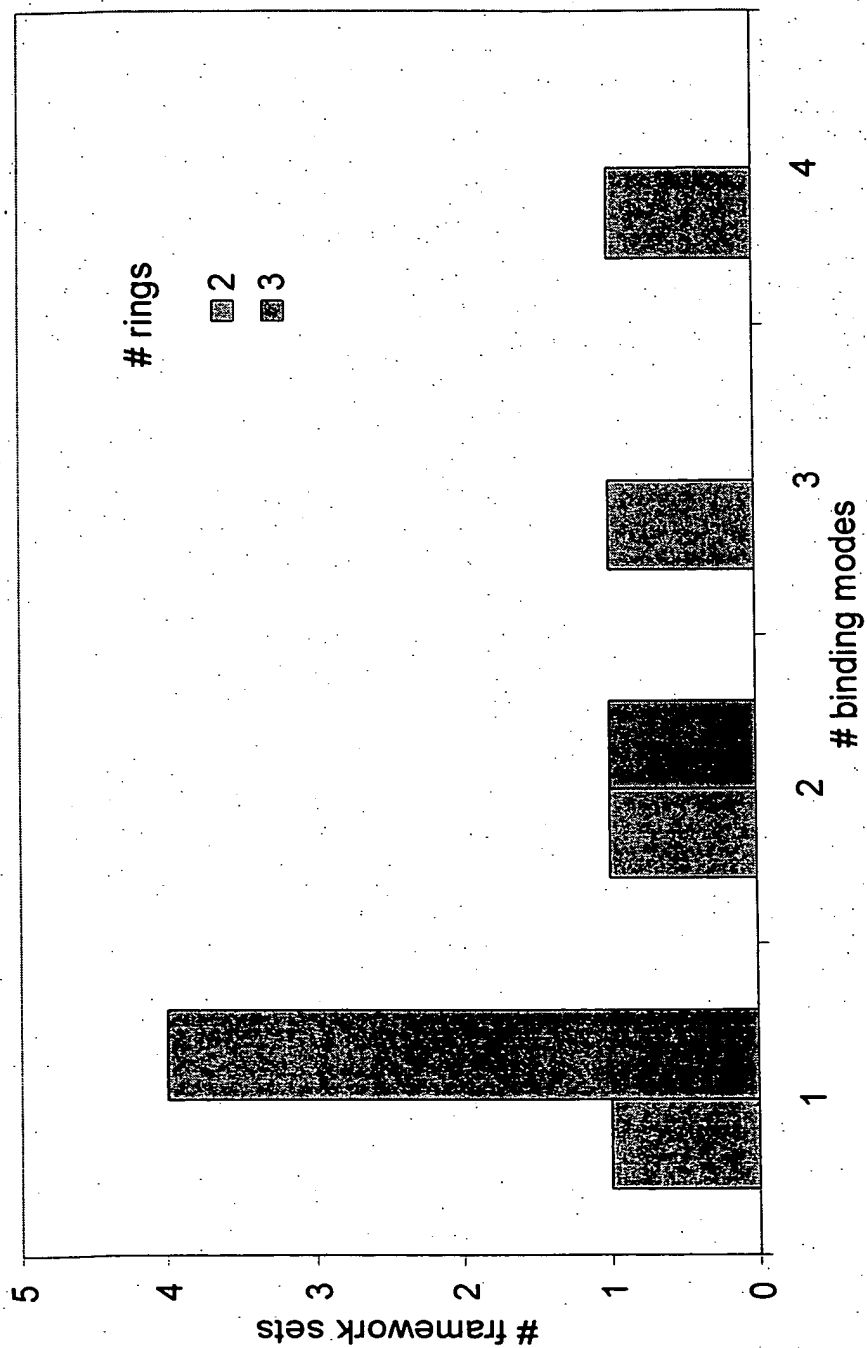


FIG. 10

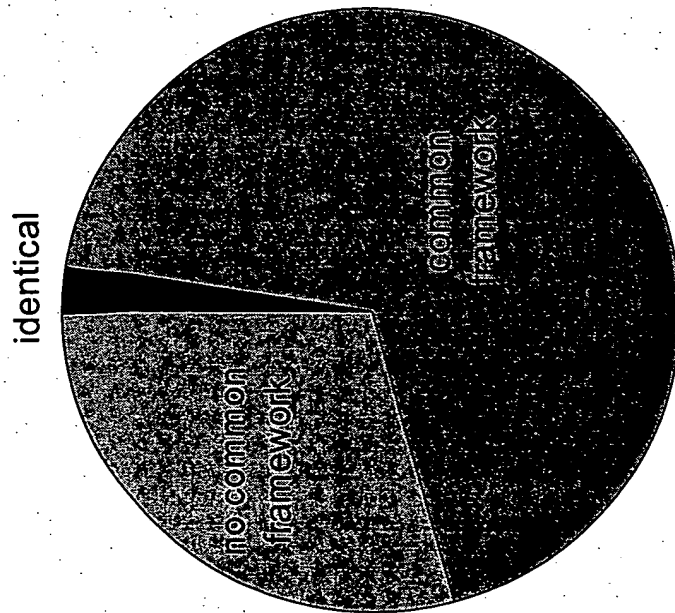


FIG. 11

Applicant(s): Guy Bemis, Paul Caron, Brian Hare  
and W. Patrick Walters  
MOLECULAR MODELING METHODS

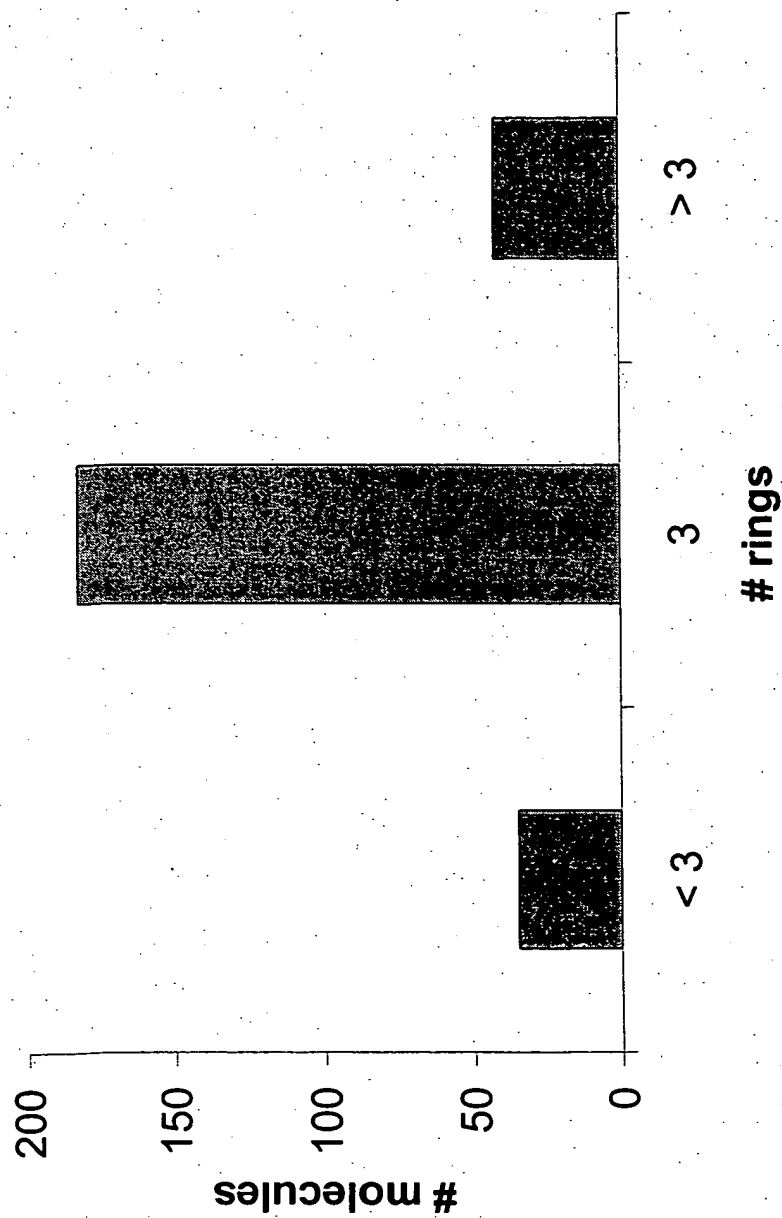
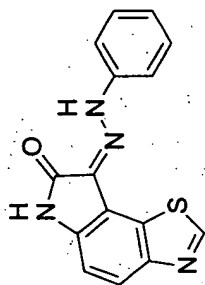
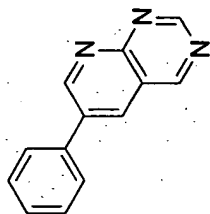


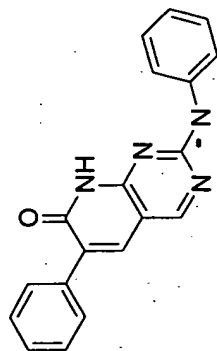
FIG. 12



10



9



8

FIG. 13